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The enhancement of luminescence in ion implanted Si quantum dots in SiO₂ matrix by means of dose alignment and doping

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The system of Si quantum dots imbedded into SiO₂ matrix (SiO₂:Si) is very promising one for many modern micro- and optoelectronic employments due to its compatibility with common silicon technology. The ion implantation is one of the most suitable and common method for the production of such a system [1–3]. Because of small thickness of implanted layers, the problem of the luminescence enhancement for the SiO₂:Si system is important. There is one apparent way to resolve this problem — the increase of excess concentration C_{Si} of Si by the increase of Si⁺ dose. But this way is not a simple one. Indeed, the luminescence intensity must increase with areal density N_S of Si nanoinclusions (NI) with appropriate for quantum confinement sizes. Generally speaking, it is not clear if the N_S would increase proportionally to C_{Si} : with increase of C_{Si} not only N_S but also average sizes of NI may grow, as well. Besides, the relation between dose and C_{Si} value is not simple due to complicated processes that must be taken into account at high doses of ion implantation (sputtering, swelling, ion mixing, change of composition, etc). It is evident that at sufficiently high doses, the sizes of NI will be so large that quantum confinement (and, hence luminescence related with quantum dots) reduction will occur. Therefore, one should look forward that, even at favourable conditions, the dose dependence of luminescence should not be monotonous one.

Recently, we have established once more factor that enhances the photoluminescence (PL) in SiO₂:Si system, namely, the additional doping of system by phosphorous implantation [4, 5]. The mechanisms of phosphorous influence on PL properties are unknown, although some assumptions were suggested in [4, 5].

In this work, we investigated, both theoretically and experimentally, the relation between Si⁺ dose and PL intensity and carried out some experiments to clear out the mechanisms of phosphorous doping influence on PL.

The thermal oxidized samples of Si with oxide thickness of 300 nm were used. The room temperature ion implantation was carried out at energy $E = 150$ keV and at doses $\phi = 1 \times 10^{17}$ to 1×10^{18} cm⁻². After implantation, the samples were annealed at 1000 °C, 2 h. Part of the samples was additionally implanted by P⁺ with the same E at $\phi = 1 \times 10^{16}$ cm⁻². The PL was measured at room temperature at $\lambda = 488$ nm (Ar laser). The Raman spectra were determine at oblique beam incidence to decrease the substrate signal. The PL peak at approximately ~ 800 nm that is characteristic one for the SiO₂:Si system [1–3] is observed for all the implanted samples. The position of the peak is about the same with exception of the largest doses ($\phi > 4 \times 10^{17}$ cm⁻²), for which it is shifted towards the red site. As it was expected, the PL intensity nonmonotonously changes with dose.

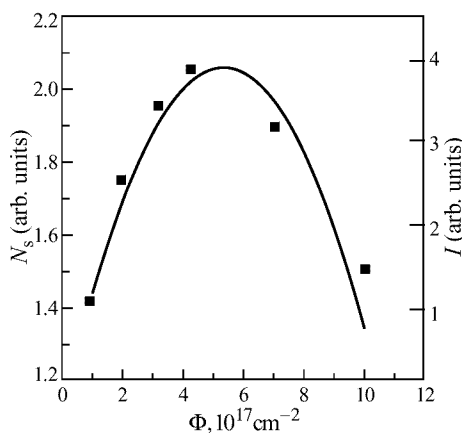


Fig. 1. The dependence of surface concentration of silicon nanoinclusions (curve) and integral PL intensity (points) on Si dose.

In order to interpret these data, we have carried out the calculation of N_S according to the following assumption. The concentration of NI at any depth is changed proportionally to the volume occupied by the excess (superstoichiometric) concentration of Si atoms until NI is overlapped at this depth. The overlapping means that volume α occupied by excessive Si atoms becomes equal to α^* , where α^* is varied parameter, α^* is near 0.5. This assumption must be fulfilled if mean size of NI does not change and if all (or constant part of) the excess Si atoms enter into NI during annealing. Then the relative value of N_S at any dose is determined by the integration over the depths for which $\alpha < \alpha^*$. The α values versus depths were computed by Monte Carlo method (TRIDIN code [6]) taking into account pointed out processes.

In Fig. 1 the calculated dose dependence of N_S (curve) is presented together with experimental values of integral PL peak intensity (points). Good accordance between experimental and calculated data speaks in favour of that above pointed assumption is right. This means that NI average size, indeed, is not changed with dose at $\phi < 4 \times 10^{17} \text{ cm}^{-2}$. The data of Raman spectra show that Raman shift is not altered until $\phi > 4 \times 10^{17} \text{ cm}^{-2}$. This fact serves as additional evidence of NI size constancy. As it follows from PL peak position and from Raman shift, average size of NI is about 4–5 nm.

The theoretical estimation shows that at sufficiently high supersaturation and providing that the complexes composed of two Si atoms serve as nucleus of NI, the concentration of NI should be approximately proportional to the excess Si atom density at not too large doses.

Other factor that enhances the PL is phosphorous doping (Fig. 2). Three mechanisms can provide this enhancement. First, the influence of P on processes of NI nucleation and growth. Second, the passivation of defects (dangling bonds) in NI or on their surfaces. (These defects may serve as nonradiative centres of recombination reducing the PL.) The third mechanism is related with the change of radiative interband transitions between quantum dot levels when the electron of donor atom fills in the level in conduction band of quantum dot. (Even at lowest Si dose, the concentration of P atoms at $\Phi_p = 1 \times 10^{16} \text{ cm}^{-2}$ is enough to provide more than one donor atom into each NI).

It is shown that intermediate annealing at 1000 °C, 2 h does not influence on the degree of PL enhancement by the phosphorous doping. It permits to deny the first mechanism of PL

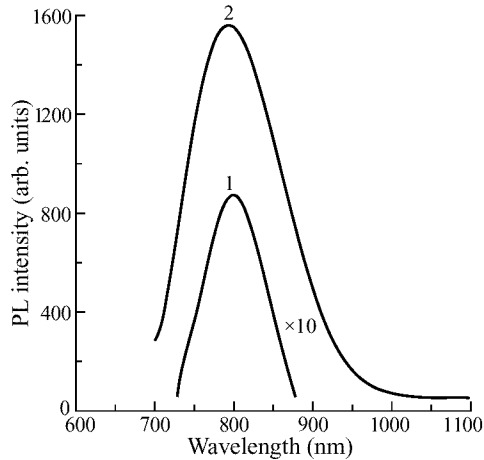


Fig. 2. The PL spectra without (1) and with (2) phosphorus doping.

enhancement. In order to check the rest two mechanisms, we have measured the relations of PL intensities with/without phosphorous implantation in dependence of excitation light power. The relation occur to be lower at small powers and then it goes to constant value. This may be explained as follows. At low excitations, the stationary density of excited electrons on the first quantum level is small, and therefore the role of doping is large. As the steady-state density of excited electron grows, the role of additional electrons related with doping is decreased. At high light power, the relation of intensities does not tend to unity. Hence, the third mechanism (passivation) becomes apparently dominating one at high excitation power.

Thus, the PL intensity can be enhanced both by Si dose alignment and by additional phosphorous doping. The influence of acceptor doping is now under investigation.

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